A SAS RESPONSE SURFACE
DESIGN AND ANALYSIS PACKAGE

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ABSTRACT

Two SAS procedures have been developed to deal with quasi-ideal response surface analysis of experimental data. The RSDESIGN procedure generates three classes of optimal experimental designs allowing the user to run experiments with almost any number of factors. The experiments may also be run in blocks. The RSANALYSIS procedure analyzes the experimental measurements coinciding with the generated design points. RSANALYSIS allows the user to model the experimental results and to determine experimental settings which jointly optimize many responses.

INTRODUCTION

In scientific experimentation it is often necessary to find combinations of settings of some factors which yield optimum characteristics (such as quality or strength) for some end product. The factors may be for example amounts of compounds used to make the product or some measurements describing conditions under which the product is made, such as temperature. The experimenter may test all possible combinations of settings to find out which combination is best. This becomes very expensive and time consuming especially when the factors are essentially of a continuous nature.

By fitting a quadratic or second-order polynomial response surface model (i.e. \( Y = a_0 + a_1 X_1 + a_2 X_2 + \ldots + b_1 X_1 X_2 + b_2 X_1 X_3 + \ldots + \epsilon \)) to some carefully chosen factor levels \((X_1, X_2, \ldots)\), interpolation can be used to estimate responses that would be obtained when the factors were set at other levels not actually run in the experiment. Thus optimum factor levels can be found with a great savings in the number of trials. The response surface model has been found to adequately fit responses in a wide variety of applications.

The Response Surface Design and Analysis Package is used for designing and analyzing such experiments. The user may select one of three major types of experimental designs to use and any number of factors may be used. The RSANALYSIS procedure features a method for constrained optimization of several responses that require a minimum of user specifications and allows the user to control how much weight should be given to each response when compromises are necessary in joint optimization.

RSDESIGN PROCEDURE

There are several methods in the statistical literature for constructing an efficient experimental design for quadratic or second-order polynomial response surface estimation. The RSDESIGN procedure uses three algorithms to automatically generate the sequence of design points (3-factor combinations) according to the user’s need for (1) economizing on the number of experimental runs, (2) achieving a certain precision for predicted responses, or (3) restricting the number of levels for some factor. Different designs or different parameters used in constructing a given design can be used to achieve the different aims. The procedure can produce blocked as well as unblocked designs and it outputs a random number to be used in randomizing the order of experimental runs. The procedure is run using statements of the following form:

```sas
PROC RSDESIGN options_and_parameters;
  FACTORS name=low TO high ...
  name=low TO high;
```

The FACTORS statement specifies the names to be used for the factors (independent variables) and the low and high levels for each factor. For two designs, the low and high values are the actual lower and upper limits for the design points; for the remaining design (CCD, see below) the low and high values are the actual lower and upper limits for the majority of design points (those in the factorial design portion) but some additional points (axial points) fall outside this range.

A parameter called METHOD controls how different design types are selected. It may have the following values: METHOD=CCD (central composite design: the default), METHOD=LEVELS (3-level design), or METHOD=MINIMUM (minimum-point design).

The central composite design is due to G.E.P. Box and K.B. Wilson (1951). It uses 3 levels for each factor and allows the experimenter to test a factor over a broad range while maintaining enough points on the interior of the range to assess the fit of the quadratic model. The design can be used for any number of factors and the user can specify the
degree of fractional replication for the factorial portion or list this default. RSDESGN attempts to generate designs that are rotatable, of uniform precision, and orthogonally blocked. Rotatability means that for all design points at a fixed distance from the center, the precision of predicted responses is the same; uniform precision means that the precision of predicted responses at center points is the same as that of any point at a distance of one standardized unit from the center. When these properties cannot be achieved (e.g. when the user overrides default parameters to meet some special need), the procedure informs him of the extent that rotatability, uniform precision, or orthogonal blocking have been sacrificed.

The 3-level design was formulated by G.E.P. Box and D.W. Behnken (1960). This design is approximately rotatable and allows the researcher to study continuous factors using a minimum number of levels for each factor.

The minimum-point design of M.J. Box and N.R. Draper (1974) is constructed to be optimum subject to the condition that the design contains the fewest possible number of points to fit the parameters of the quadratic equation: some center points are added to this minimum design to assess lack of fit of the model. It is a 3-level design like the CCD.

The first two designs can be blocked for most values of f, the number of factors. This allows the experiments to be run in smaller batches requiring homogeneous test conditions only within each block. For the CCD and MINIMUM designs, the user can specify the number of center points to use or a default value is used. The user can optionally specify how the axial points in the CCD are chosen and can specify a parameter called SEED to control the randomization sequence so it can be recreated. An option, BLOCK, is specified to get a blocked design.

The output of RSDESGN consists of a SAS dataset containing the design points, blocking label (if any), a random number called RANDOM, and a variable _TYPE_ indicating the types of design points (factorial, axial, center, other). In the following example, an unblocked 3-level design is generated for 3 factors.

```
PROC RSDESGN METHOD=LEVELS; SEED=13;
  FACTORS GRIND=4 TO 12 TEMP=1400 TO 1460 PUSH=10 TO 30;
  RANDOMIZE ORDER OF RUNS;
  PROC EDIT OUT=STDROP=Random 
    _TYPE_; BY RANDOM;
  PROC PRINT TITLE EXPERIMENTAL PLAN;
```

The output is:

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EXPERIMENTAL PLAN

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</table>
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RSANALYSIS PROCEDURE

The RSANALYSIS procedure performs general quadratic response surface analysis to help the researcher model his experimental outcome as a function of input parameters or factors and to estimate the combination of input parameters that yields the best set of responses. The procedure will do the following:

1. Perform an analysis of variance for each full model
2. Fit restricted models
3. Print predicted responses and confidence limits
4. Fit models by adding terms in a stepwise fashion
5. Plot contour graphs and X-Y graphs
6. Find factor levels that optimize general functions of the response variables. Any number of responses may be optimized jointly or singly and the user may specify how much weight should be given to each response when compromises are necessary in joint optimization.

Many of these tasks are accomplished by using other SAS procedures (e.g. BYPROC, GLM, RSREG, STEPWISE, PLOT) in which case RSANALYSIS serves as an interpreter so the user can get the analyses using a minimum of statements. For tasks 5 and 6 above, RSANALYSIS stores the symbolic prediction equation.
for each response to efficiently construct series of points for plotting and to search for optimum factor combinations.

RSANALYSIS has as input a SAS dataset containing the factor levels (e.g. from RDS DESIGN), corresponding response determinations, and blocking label, if any. It is run using statements like the following:

PROC RSANALYSIS OPTIONS;
FACTORS name1 name2 ... nameN;
RESPONSES response1 response2 ... responseM;
MODEL ... ;
CONTOUR ... ;
GRAPH ... ;
OPTIMIZE ... ;

The FACTORS statement names the factors or independent variables. RESPONSES names all the response (dependent) variables. There may be zero or more MODEL statements and any number of CONTOUR, GRAPH, and OPTIMIZE statements. Unless told otherwise, RSANALYSIS invokes the RSREG procedure (Sall, 1980) to print a detailed analysis of variance table and perform a lack of fit test, using the replicated center points to get an estimate of "pure error". When the experiment is blocked, RSANALYSIS automatically constructs blocking indicator variables to be used with the different SAS procedures and the instructions to these procedures are modified accordingly to handle the blocking.

If there are no MODEL statements, a full second-order polynomial model is fitted for each response variable. Optionally, a MODEL statement specifies which terms are to be included in each response model, for example:

MODEL Y1=A C A&B C**2;
MODEL Y2=LINEAR;
MODEL Y3=LINEAR CROSSPRODUCT;

A MODEL statement can be applied to all responses by using e.g. "MODEL _ALL_LINEAR QUADRATIC;".

The CONTOUR statement causes RSANALYSIS to set up instructions to the RSP procedure (Chillko, in SAS Supplemental Guide) to get contour plots, for example:

CONTOUR; or
CONTOUR list of response variables;
RANGES ... ; PLOT ... ; see RSP documentation;

When simply "CONTOUR;" is given, plots will be produced for all response variables.

The GRAPH statement is used to plot one factor (X-variable) versus one response (Y-variable) holding the levels of other factors constant or varying them to get separate graphs. PROC PLOT is used to do this after RSANALYSIS sets up the necessary instructions. The GRAPH statement may have one of two forms:

GRAPH response=factor=low TO high
   HOLDING X2=0 X3=10 TO 30
   X4=1 TO 9 BY 2;
or
GRAPH response=factor HOLDING .... ;

When the second form is used, the lower and upper limits for the factor are taken as the actual limits occurring in the data.

OPTIMIZATION

In finding the combination of input parameters or factor settings that is "best" in terms of yielding the best possible end product or response, the following considerations arise:

1. There may be many objectives to optimize, some of them conflicting.

2. The optimum factor levels must be constrained to be in reasonable limits.

3. An objective is easy to formulate when only what describes "good quality" needs to be specified. It is more demanding to require the user to specify how good is "good". For example, if one objective is a long life expectancy of a product, the user would rather specify "the longer the better" than to have to quantify the utility of the product per unit increase of life length.

4. When objectives conflict, as when combinations yielding a long product life also result in a high production cost, the user should be able to rate the relative importance of the two objectives to get the best compromise set of input parameters or he should be able to get, for example, the set of parameters resulting in a medium life length at medium cost.

The RSANALYSIS procedure incorporates a ranking method to make such decisions in
finding optimum levels. This method is best illustrated by the following example. Suppose that an athletic contest is held among 10 students, for two events — broad jumping and high jumping. The teacher does not know how to weigh broad jumping and high jumping capabilities of a student to get an overall score, so he ranks each student’s jump in the set of all students jumps, separately for broad jump and high jump. Student A ranks first in broad but third in high jump. Student B ranks second for both jumps. If both jumps receive equal weight, the teacher rates the students both with an average ranking of 2. However, if he considers high jumping to be twice as important in some sense, the first student has a weighted average score of \((1+2+3)/(1+2)=2.33\) and the second student has a weighted score of \((1+2+2)/(1+2)=2\) and the teacher gives the award to student B.

RBANALYSIS examines objectives for combinations of factor levels of interest to the user and applies this ranking procedure to rate the combinations with regard to all objectives. The objective functions specified by the user need only order the responses in increasing quality. The unweighted analysis is always performed and the user may specify any number of sets of weights to use in weighted analyses. In each analysis, the best 20 (by default) combinations are listed. As a special case one objective can receive all the weight so the user can get the best combinations with respect to that objective alone; he can then examine the list of all other predicted responses for each of the best 20 or so combinations listed in order of decreasing quality of the objective receiving all the weight. This will allow him to choose a "best" compromise combination.

The OPTIMIZE statement along with the associated OBJECTIVES statement and the optional ACCEPT and WEIGHTS statements tell RBANALYSIS to estimate combinations of factor levels yielding joint optimum or "compromised" joint optimum predicted responses. The statements have the following format:

```
OPTIMIZE x1=low TO high BY incr 
x2=value x3=low TO high / optional parameters;
```

or

```
OPTIMIZE;
ACCEPT expression;
OBJECTIVES name1: function1 
    name2: function2 ... 
    nameq: functionq;
WEIGHTS w1 w2 ... wq ... 
    w1 v2 ... vq;
```

The ranges in OPTIMIZE specify the region of independent variables to examine for optimum responses. If omitted, the range occurring in the data used to fit the response surfaces is used. The optional ACCEPT statement allows the user to specify any valid SAS expression that a predicted response must satisfy before it is even considered in the search. e.g. ACCEPT Y1>100&Y2<3;

The OBJECTIVES statement specifies functions of the responses such that a low value of the function is considered desirable. Example: suppose for a response Y1, high values are desirable, and for Y2, values close to 10 are desirable. One OBJECTIVES statement might be "OBJECTIVES A: Y1; B:ABS(Y2-10)". For each WEIGHTS statement, the final stage of the analysis is repeated and the best combinations of independent variable settings, with respect to the weighted ranking of the objective functions, are listed.

**REFERENCES**


**ACKNOWLEDGEMENT**

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STATISTICS (NON-GLM)

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